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QUANTUM DESIGN OF MATERIALS ON THE CRAY T3D, L.H. Yang, Lawrence Livermore National Laboratory, Livermore, CA*

The prospects for realistic simulations of cohesive, structural, mechanical and electronic properties of materials have improved significantly in recent years. Density-functional theory (DFT) in the local-density approximation (LDA) has yielded accurate results for many materials problems ranging from the bulk to the surface. Furthermore, the development of new numerical algorithms and the introduction of massively parallel-processing architectures, now makes feasiblethe *ab initio* treatment of technologically important materials.

The parallelization strategies of an ab initio total-energy molecular dynamics (MD) code on the Cray T3D using Shared Memory Access library (SHMEM) will be described. In particular, we have implemented the following two features in our parallel code. The work partition which allows the minimization of the communications and the optimization of the load balancing. The parallel I/O which speeds up 15% of the code by the number of processors. With these efforts, we have obtained high parallel efficiency up to 64 node of our *ab initio* MD code. The scalability of our code as a function of the number of nodes will be presented.

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